

# 1,4-Cyclohexanediacetic acid, dimethyl ester

<b>Inchi:</b>	InChI=1S/C12H20O4/c1-15-11(13)7-9-3-5-10(6-4-9)8-12(14)16-2/h9-10H,3-8H2,1-2H3
<b>InchiKey:</b>	BPNODYPKYHGPEF-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O4
<b>SMILES:</b>	COC(=O)CC1CCC(CC(=O)OC)CC1
<b>Mol. weight [g/mol]:</b>	228.28
<b>CAS:</b>	21810-40-2

## Physical Properties

Property code	Value	Unit	Source
gf	-400.94	kJ/mol	Joback Method
hf	-746.63	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.919		Crippen Method
mcvol	183.960	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
tb	641.42	K	Joback Method
tc	846.20	K	Joback Method
tf	372.46	K	Joback Method
vc	0.688	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.57	J/molxK	641.42	Joback Method
cpg	587.94	J/molxK	812.07	Joback Method
cpg	574.26	J/molxK	777.94	Joback Method
cpg	559.58	J/molxK	743.81	Joback Method
cpg	543.90	J/molxK	709.68	Joback Method
cpg	527.23	J/molxK	675.55	Joback Method
cpg	600.62	J/molxK	846.20	Joback Method
dvisc	0.0001901	Paxs	641.42	Joback Method
dvisc	0.0002418	Paxs	596.59	Joback Method

dvisc	0.0003198	Paxs	551.77	Joback Method
dvisc	0.0004445	Paxs	506.94	Joback Method
dvisc	0.0006584	Paxs	462.11	Joback Method
dvisc	0.0010612	Paxs	417.29	Joback Method
dvisc	0.0019188	Paxs	372.46	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21810402&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21810402&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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